Computer Simulations of Chemical and Biological Processes

Abstract: Many chemical and biological processes require the breaking and forming of chemical bonds and other quantum mechanical effects. Such processes cannot be simulated with standard classical molecular dynamics methods and require quantum mechanical methods. In many cases, the systems are so large that fully quantum mechanical calculations are not computationally practical. Such systems can be simulated using hybrid quantum /classical methods, which treat only the key regions quantum mechanically. This talk will provide an overview of hybrid quantum/classical computer simulations of chemical and biological processes. Three different types of simulations will be discussed. The first topic is mixed quantum mechanical /molecular mechanical free energy simulations of enzymes and ribozymes, which are RNA enzymes. The reactive region is treated with a quantum mechanical method such as density functional theory to allow bonds to form and break, while the remainder of the system is treated with standard classical molecular mechanical force fields. The multidimensional free energy surface is simulated with statistical methods that focus on the regions of interest. The second topic to be covered is nonadiabatic molecular dynamics simulations of photoinduced electron and proton transfer reactions. The excited electronic states of the molecule are calculated on-the-fly with a multiconfigurational quantum mechanical method during the molecular dynamics trajectory, while the solvent is treated with a molecular mechanical force field. Nonadiabatic transitions between the excited electronic states are included with a time-dependent quantum mechanical algorithm to simulate the relaxation process following photoexcitation. The third topic to be covered is electronic structure calculations of molecular systems that exhibit nuclear quantum effects and non-Born-Oppenheimer effects. Specified protons must be treated quantum mechanically on the same level as the electrons in order to calculate accurate molecular properties. Supercomputers have been essential to the success in all three of these areas.

Bio: Dr. Sharon Hammes-Schiffer is the Swanlund Chair and Professor in the Department of Chemistry at the University of Illinois at Urbana-Champaign. She received her B.A. in Chemistry from Princeton University (1988) and her Ph.D. in Chemistry at Stanford University (1993). She was a postdoctoral research scientist at AT&T Bell Laboratories (1993-95) and was on the faculties of the University of Notre Dame (1995-2000) and The Pennsylvania State University (2000-2012). Dr. Hammes-Schiffer is a Fellow of the American Physical Society, American Chemical Society, American Association for the Advancement of Science, and Biophysical Society. She is a member of the American Academy of Arts and Sciences, the U.S. National Academy of Sciences, and the International Academy of Quantum Molecular Science. She was the Deputy Editor of *The Journal of Physical Chemistry B* and is currently the Editor-in-Chief of *Chemical Reviews*. She has also served as Chair of the Theoretical Subdivision and the Physical Division of the American Chemical Society and is a member of the Basic Energy Sciences Advisory Committee. She has over 190 scientific publications and has given more than 270 invited talks.

Dr. Hammes-Schiffer's research centers on the investigation of charge transfer reactions, dynamics, and quantum mechanical effects in chemical, biological, and interfacial processes. Her work encompasses the development of analytical theories and computational methods, as well as applications to a wide range of experimentally relevant systems. Her biological simulations have elucidated the roles of hydrogen tunneling, electrostatics, and protein motion in enzyme catalysis and have provided insights into the fundamental mechanisms of ribozyme catalysis. Her calculations of proton-coupled electron transfer in molecular electrocatalysts and photoinduced dynamical processes are guiding the design of more effective catalysts for energy conversion processes essential to solar energy devices.